

4-(Chloromethyl)-2-ethoxy-1,3,2lambda⁵-dioxaphospholan-2-one

67554-11-4 | DTXSID50791173

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 8.50e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.16e-01

Confidence level: 7.04e-01

Nearest Neighbors from the Training Set

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Dichlorvos

Measured: 4.05e-02

Predicted: 3.21e-02

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Phosphoric acid, 2-chloroethenyl diethyl ester

Measured: 4.66e-02

Predicted: N/A

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Tris(2-chloroethyl) phosphate

Measured: 2.45e-02

Predicted: 2.74e-02

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Cyclophosphamide

Measured: 1.53e-01

Predicted: 8.08e-02